2'-Deoxyadenosine, 3'-O-TBDMS

Inchi: InChI=1S/C16H27N5O3Si/c1-16(2,3)25(4,5)24-10-6-12(23-11(10)7-22)21-9-20-13-14(17
InchiKey: RZJNKNBLADNWHG-PQDIPPBSSA-N
Formula: C16H27N5O3Si
SMILES: CC(C)(C)[Si](C)(C)OC1CC(n2cnc3c(N)ncnc32)OC1CO
Mol. weight [g/mol]: 365.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.079		Crippen Method
rinpol	2731.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R246727&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices